Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:38 AM GMT

PDB ID	:	3MGU
Title	:	Saccharomyces cerevisiae Tpa1
Authors	:	Henri, J.; Rispal, D.; Bayart, E.; van Tilbeurgh, H.; Seraphin, B.; Graille, M.
Deposited on	:	2010-04-07
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

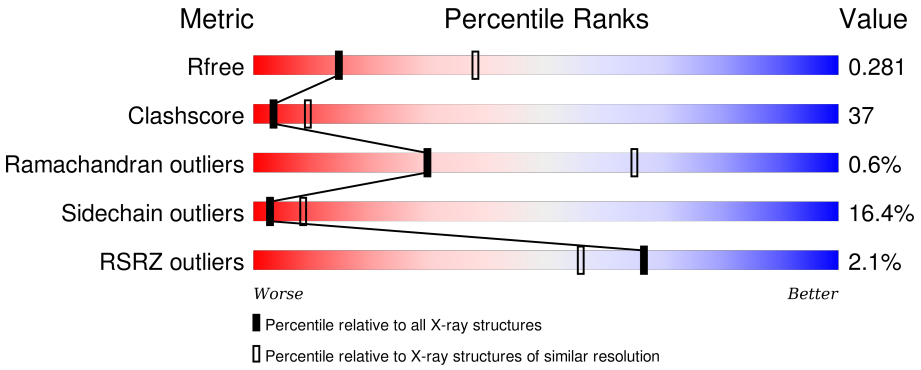
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	644	2% 36% 36% 10% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4406 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PKHD-type hydroxylase TPA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4372	2813	730	816	13			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

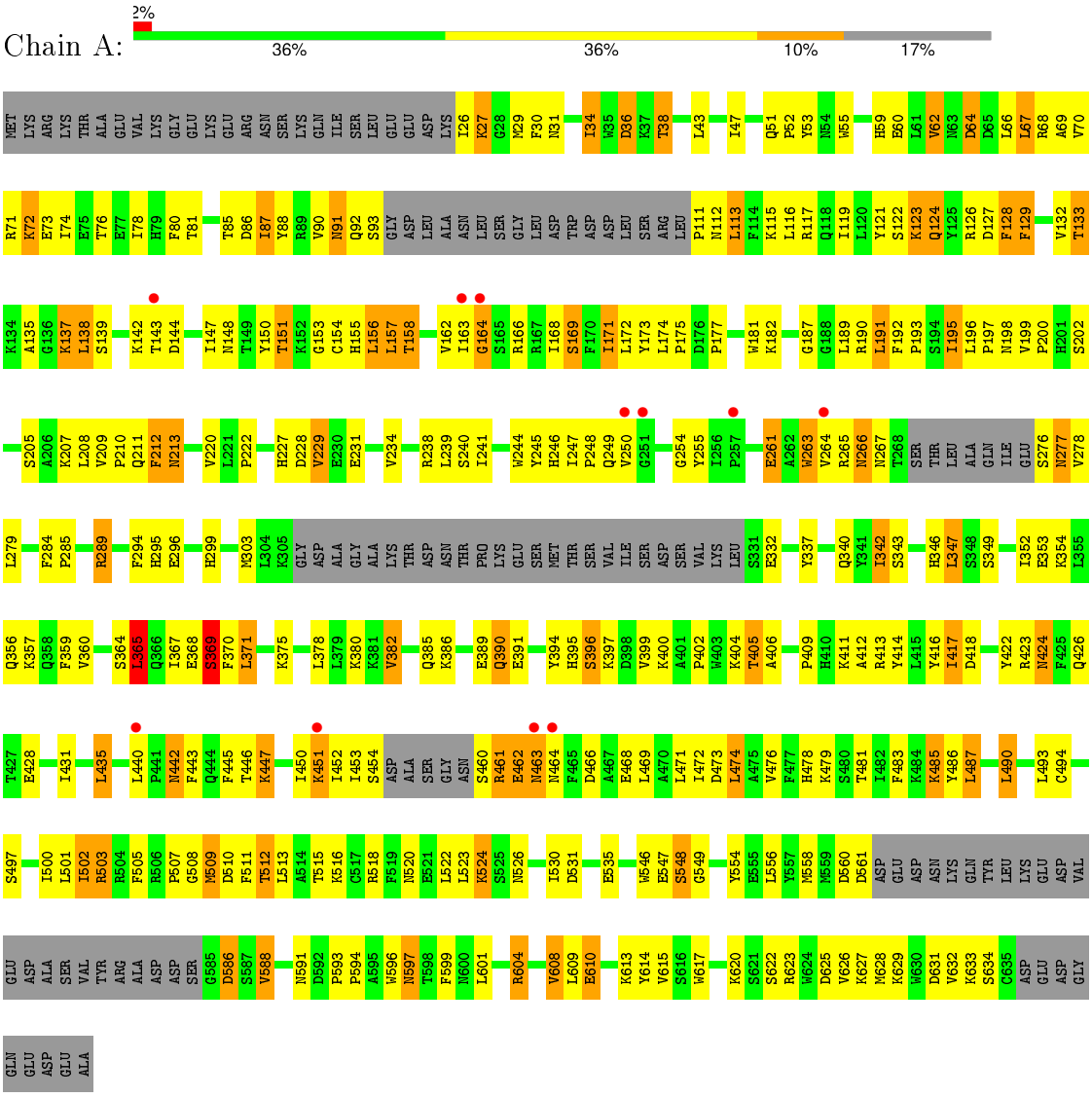
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PKHD-type hydroxylase TPA1

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	81.18Å 104.84Å 205.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.80 46.85 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.92-2.80) 99.3 (46.85-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.296 0.231 , 0.281	Depositor DCC
R_{free} test set	1095 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.861	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 22112 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4406	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.34	0/4480	0.54	1/6048 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	LEU	CA-CB-CG	6.87	131.10	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4372	0	4307	318	0
2	A	1	0	0	0	0
3	A	33	0	0	3	0
All	All	4406	0	4307	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:HA	1:A:409:PRO:HG3	1.28	1.15
1:A:424:ASN:HD21	1:A:426:GLN:HE21	1.04	0.97
1:A:289:ARG:HH11	1:A:289:ARG:HG2	1.26	0.96
1:A:371:LEU:H	1:A:597:ASN:HD21	1.08	0.96
1:A:175:PRO:HD2	1:A:212:PHE:HA	1.50	0.94
1:A:507:PRO:HA	1:A:615:VAL:HG12	1.50	0.93
1:A:69:ALA:HB1	1:A:112:ASN:HD21	1.37	0.89
1:A:461:ARG:HD3	1:A:461:ARG:H	1.37	0.88
1:A:535:GLU:OE1	1:A:604:ARG:HD2	1.74	0.87
1:A:395:HIS:CD2	1:A:397:LYS:HG2	2.10	0.86
1:A:200:PRO:HG2	1:A:409:PRO:HD2	1.58	0.86
1:A:479:LYS:HG3	1:A:500:ILE:HD12	1.59	0.84
1:A:31:ASN:HA	3:A:668:HOH:O	1.79	0.81
1:A:289:ARG:HH11	1:A:289:ARG:CG	1.97	0.77
1:A:337:TYR:O	1:A:340:GLN:HG2	1.85	0.76
1:A:442:ASN:ND2	1:A:445:PHE:H	1.83	0.75
1:A:285:PRO:HG3	1:A:416:TYR:CZ	2.21	0.75
1:A:87:ILE:O	1:A:157:LEU:HD22	1.86	0.75
1:A:417:ILE:HG23	1:A:502:ILE:HG12	1.69	0.74
1:A:91:ASN:HD21	1:A:151:THR:HG22	1.50	0.73
1:A:394:TYR:HD1	1:A:509:MET:SD	2.10	0.73
1:A:181:TRP:H	1:A:211:GLN:HE22	1.36	0.73
1:A:394:TYR:CD1	1:A:509:MET:SD	2.82	0.72
1:A:177:PRO:HG3	1:A:212:PHE:CE2	2.23	0.72
1:A:424:ASN:ND2	1:A:426:GLN:HE21	1.84	0.71
1:A:69:ALA:CB	1:A:112:ASN:HD21	2.03	0.71
1:A:27:LYS:HE3	1:A:27:LYS:N	2.06	0.71
1:A:560:ASP:O	1:A:561:ASP:HB2	1.89	0.71
1:A:138:LEU:HD23	1:A:168:ILE:HD12	1.73	0.69
1:A:356:GLN:O	1:A:360:VAL:HG23	1.92	0.69
1:A:126:ARG:HB3	1:A:138:LEU:HD13	1.73	0.69
1:A:535:GLU:OE2	1:A:627:LYS:HE2	1.92	0.69
1:A:169:SER:HB2	1:A:244:TRP:NE1	2.09	0.68
1:A:220:VAL:O	1:A:220:VAL:HG12	1.92	0.68
1:A:157:LEU:HA	1:A:228:ASP:HB2	1.76	0.67
1:A:166:ARG:HD3	1:A:244:TRP:CD1	2.29	0.67
1:A:483:PHE:CE2	1:A:487:LEU:HD23	2.28	0.67
1:A:277:ASN:HD22	1:A:277:ASN:C	1.98	0.67
1:A:67:LEU:HD21	1:A:172:LEU:HD21	1.77	0.66
1:A:413:ARG:O	1:A:510:ASP:HA	1.94	0.66
1:A:371:LEU:H	1:A:597:ASN:ND2	1.90	0.66
1:A:511:PHE:HB3	1:A:614:TYR:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:O	1:A:478:HIS:HD2	1.79	0.65
1:A:162:VAL:HG22	1:A:220:VAL:HG13	1.79	0.65
1:A:156:LEU:HB3	1:A:229:VAL:HG13	1.76	0.65
1:A:51:GLN:HG2	1:A:52:PRO:HA	1.77	0.65
1:A:385:GLN:HE22	1:A:463:ASN:ND2	1.95	0.65
1:A:395:HIS:HD2	1:A:397:LYS:HG2	1.59	0.64
1:A:193:PRO:HD3	1:A:205:SER:OG	1.97	0.64
1:A:522:LEU:HD12	1:A:522:LEU:H	1.62	0.64
1:A:285:PRO:HG3	1:A:416:TYR:CE1	2.32	0.64
1:A:494:CYS:HB2	1:A:633:LYS:HG2	1.79	0.64
1:A:402:PRO:HB2	1:A:417:ILE:HD13	1.80	0.63
1:A:73:GLU:OE2	1:A:111:PRO:HB2	1.98	0.63
1:A:505:PHE:O	1:A:622:SER:HB3	1.98	0.63
1:A:442:ASN:HD22	1:A:445:PHE:H	1.47	0.63
1:A:139:SER:HB2	1:A:248:PRO:HA	1.81	0.63
1:A:208:LEU:HD23	1:A:208:LEU:H	1.62	0.62
1:A:123:LYS:HE2	1:A:127:ASP:OD2	1.99	0.62
1:A:546:TRP:CE3	1:A:594:PRO:HG2	2.36	0.61
1:A:558:MET:HB3	1:A:588:VAL:HA	1.82	0.61
1:A:47:ILE:HD12	1:A:132:VAL:O	2.00	0.61
1:A:353:GLU:O	1:A:357:LYS:HD3	2.01	0.61
1:A:187:GLY:O	1:A:238:ARG:NH1	2.33	0.61
1:A:460:SER:HB2	1:A:462:GLU:HG2	1.83	0.60
1:A:371:LEU:N	1:A:597:ASN:HD21	1.91	0.60
1:A:71:ARG:HG2	1:A:72:LYS:HZ1	1.66	0.60
1:A:353:GLU:HA	1:A:356:GLN:HE21	1.66	0.60
1:A:507:PRO:HA	1:A:615:VAL:CG1	2.27	0.60
1:A:91:ASN:ND2	1:A:151:THR:HG22	2.16	0.60
1:A:277:ASN:HD22	1:A:278:VAL:N	2.00	0.60
1:A:446:THR:O	1:A:450:ILE:HD13	2.01	0.60
1:A:447:LYS:HE3	1:A:451:LYS:NZ	2.16	0.60
1:A:73:GLU:CD	1:A:111:PRO:HB2	2.22	0.59
1:A:26:ILE:HG13	1:A:27:LYS:CE	2.32	0.59
1:A:142:LYS:HD3	1:A:246:HIS:ND1	2.17	0.59
1:A:52:PRO:HG3	1:A:205:SER:OG	2.02	0.59
1:A:209:VAL:HG23	1:A:209:VAL:O	2.03	0.59
1:A:80:PHE:HD1	1:A:92:GLN:O	1.86	0.59
1:A:74:ILE:HG12	1:A:78:ILE:HD12	1.85	0.58
1:A:202:SER:O	1:A:413:ARG:NH1	2.36	0.58
1:A:174:LEU:N	1:A:175:PRO:HD3	2.17	0.58
1:A:289:ARG:HD2	1:A:629:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HA	1:A:70:VAL:HG22	1.85	0.58
1:A:26:ILE:N	1:A:27:LYS:HZ1	2.01	0.58
1:A:29:MET:HA	3:A:657:HOH:O	2.04	0.58
1:A:133:THR:HG21	1:A:168:ILE:CD1	2.34	0.58
1:A:418:ASP:HB3	1:A:501:LEU:CD2	2.33	0.58
1:A:386:LYS:HZ3	1:A:464:ASN:HA	1.69	0.58
1:A:461:ARG:N	1:A:461:ARG:HD3	2.12	0.57
1:A:395:HIS:HD2	1:A:397:LYS:H	1.52	0.57
1:A:162:VAL:HG12	1:A:162:VAL:O	2.04	0.57
1:A:520:ASN:HB3	1:A:523:LEU:HG	1.86	0.57
1:A:370:PHE:HD2	1:A:371:LEU:HD13	1.69	0.57
1:A:60:GLU:HA	1:A:213:ASN:O	2.04	0.56
1:A:64:ASP:O	1:A:68:ARG:HG3	2.04	0.56
1:A:72:LYS:O	1:A:76:THR:HG23	2.05	0.56
1:A:74:ILE:HG23	1:A:78:ILE:HD12	1.87	0.56
1:A:364:SER:HA	1:A:601:LEU:O	2.05	0.56
1:A:303:MET:SD	1:A:485:LYS:HD3	2.45	0.56
1:A:36:ASP:OD1	1:A:38:THR:HG23	2.06	0.56
1:A:390:GLN:HG3	1:A:391:GLU:H	1.70	0.56
1:A:121:TYR:CD2	1:A:143:THR:HG22	2.40	0.56
1:A:196:LEU:HB2	1:A:199:VAL:HB	1.87	0.56
1:A:36:ASP:C	1:A:36:ASP:OD1	2.44	0.56
1:A:386:LYS:O	1:A:390:GLN:HB3	2.06	0.56
1:A:342:ILE:HG13	1:A:343:SER:N	2.20	0.56
1:A:453:ILE:O	1:A:454:SER:CB	2.53	0.56
1:A:195:ILE:O	1:A:196:LEU:HG	2.06	0.55
1:A:91:ASN:HD21	1:A:151:THR:CG2	2.19	0.55
1:A:342:ILE:HD11	1:A:346:HIS:HB2	1.89	0.55
1:A:174:LEU:HD21	1:A:241:ILE:HD12	1.87	0.55
1:A:547:GLU:HA	1:A:548:SER:OG	2.06	0.55
1:A:137:LYS:HG2	1:A:254:GLY:HA3	1.88	0.55
1:A:169:SER:HB2	1:A:244:TRP:HE1	1.70	0.54
1:A:522:LEU:N	1:A:522:LEU:HD12	2.23	0.54
1:A:546:TRP:O	1:A:593:PRO:HB3	2.06	0.54
1:A:173:TYR:HB3	1:A:175:PRO:HD3	1.88	0.54
1:A:513:LEU:O	1:A:515:THR:HG23	2.08	0.54
1:A:424:ASN:HD21	1:A:426:GLN:NE2	1.88	0.54
1:A:604:ARG:HB3	1:A:608:VAL:CG1	2.38	0.54
1:A:53:TYR:O	1:A:55:TRP:HD1	1.91	0.54
1:A:263:TRP:O	1:A:266:ASN:HB3	2.08	0.54
1:A:378:LEU:O	1:A:382:VAL:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:N	1:A:138:LEU:HD12	2.23	0.53
1:A:190:ARG:O	1:A:227:HIS:HA	2.08	0.53
1:A:173:TYR:C	1:A:174:LEU:HD22	2.29	0.53
1:A:404:LYS:HE2	1:A:418:ASP:OD2	2.09	0.53
1:A:51:GLN:HG2	1:A:52:PRO:CA	2.38	0.53
1:A:250:VAL:HA	1:A:255:TYR:CE1	2.44	0.52
1:A:163:ILE:HD11	1:A:166:ARG:CZ	2.39	0.52
1:A:157:LEU:H	1:A:157:LEU:HD22	1.74	0.52
1:A:385:GLN:OE1	1:A:463:ASN:HB2	2.09	0.52
1:A:208:LEU:H	1:A:208:LEU:CD2	2.22	0.52
1:A:390:GLN:HG3	1:A:391:GLU:N	2.23	0.52
1:A:261:GLU:HB2	1:A:265:ARG:HH12	1.75	0.52
1:A:67:LEU:HD13	1:A:174:LEU:HD13	1.91	0.52
1:A:523:LEU:N	1:A:523:LEU:HD23	2.25	0.52
1:A:197:PRO:O	1:A:198:ASN:HB2	2.10	0.52
1:A:507:PRO:O	1:A:615:VAL:O	2.27	0.51
1:A:474:LEU:HD22	1:A:478:HIS:CD2	2.45	0.51
1:A:385:GLN:HE21	1:A:389:GLU:HB3	1.75	0.51
1:A:171:ILE:HD13	1:A:173:TYR:CZ	2.46	0.51
1:A:135:ALA:HB3	1:A:168:ILE:HD11	1.92	0.51
1:A:503:ARG:HH11	1:A:503:ARG:CG	2.23	0.51
1:A:144:ASP:O	1:A:144:ASP:OD2	2.28	0.51
1:A:87:ILE:HG22	1:A:157:LEU:CD2	2.40	0.51
1:A:460:SER:HB2	1:A:462:GLU:CG	2.41	0.51
1:A:424:ASN:C	1:A:424:ASN:HD22	2.14	0.51
1:A:71:ARG:NH1	1:A:175:PRO:O	2.44	0.51
1:A:560:ASP:O	1:A:561:ASP:CB	2.57	0.51
1:A:162:VAL:HG22	1:A:220:VAL:CG1	2.40	0.51
1:A:53:TYR:OH	1:A:191:LEU:HD12	2.10	0.50
1:A:92:GLN:HA	1:A:148:ASN:ND2	2.27	0.50
1:A:92:GLN:O	1:A:93:SER:HB3	2.11	0.50
1:A:266:ASN:HD22	1:A:267:ASN:N	2.09	0.50
1:A:189:LEU:O	1:A:207:LYS:HA	2.10	0.50
1:A:142:LYS:O	1:A:142:LYS:HG2	2.11	0.50
1:A:266:ASN:ND2	1:A:266:ASN:C	2.65	0.50
1:A:497:SER:OG	1:A:631:ASP:HB2	2.12	0.50
1:A:342:ILE:HG12	1:A:347:LEU:CD2	2.42	0.50
1:A:247:ILE:O	1:A:249:GLN:NE2	2.44	0.50
1:A:138:LEU:H	1:A:138:LEU:HD12	1.76	0.50
1:A:400:LYS:N	1:A:400:LYS:HD2	2.26	0.49
1:A:276:SER:O	1:A:279:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:HG22	1:A:157:LEU:HD21	1.94	0.49
1:A:461:ARG:CD	1:A:461:ARG:H	2.18	0.49
1:A:474:LEU:HD13	1:A:626:VAL:HG21	1.95	0.49
1:A:623:ARG:NH1	1:A:625:ASP:OD2	2.46	0.49
1:A:370:PHE:CD2	1:A:371:LEU:HD13	2.47	0.49
1:A:189:LEU:HB3	1:A:208:LEU:HD21	1.95	0.49
1:A:299:HIS:CE1	1:A:485:LYS:NZ	2.81	0.49
1:A:464:ASN:O	1:A:468:GLU:CD	2.51	0.49
1:A:66:LEU:O	1:A:70:VAL:HG22	2.11	0.49
1:A:296:GLU:CD	1:A:481:THR:HG22	2.33	0.49
1:A:508:GLY:HA2	1:A:617:TRP:HD1	1.78	0.49
1:A:115:LYS:O	1:A:119:ILE:HG23	2.12	0.49
1:A:74:ILE:HD13	1:A:147:ILE:HG21	1.95	0.49
1:A:68:ARG:O	1:A:72:LYS:HB2	2.13	0.48
1:A:163:ILE:HD11	1:A:166:ARG:NH2	2.28	0.48
1:A:158:THR:HG23	1:A:409:PRO:O	2.13	0.48
1:A:70:VAL:HG21	1:A:116:LEU:HD22	1.95	0.48
1:A:494:CYS:HB2	1:A:633:LYS:CG	2.42	0.48
1:A:548:SER:HA	1:A:549:GLY:HA2	1.62	0.48
1:A:447:LYS:NZ	1:A:473:ASP:OD1	2.44	0.48
1:A:296:GLU:OE1	1:A:481:THR:HG22	2.13	0.48
1:A:359:PHE:HB2	1:A:365:LEU:HD12	1.95	0.48
1:A:511:PHE:CE2	1:A:513:LEU:HD11	2.48	0.48
1:A:85:THR:O	1:A:613:LYS:NZ	2.47	0.48
1:A:128:PHE:O	1:A:132:VAL:HG22	2.14	0.48
1:A:382:VAL:HG12	1:A:466:ASP:HB3	1.96	0.48
1:A:402:PRO:HG3	1:A:468:GLU:HG2	1.95	0.48
1:A:447:LYS:HD2	1:A:447:LYS:C	2.34	0.47
1:A:147:ILE:O	1:A:148:ASN:ND2	2.47	0.47
1:A:524:LYS:HD3	1:A:524:LYS:HA	1.65	0.47
1:A:151:THR:O	1:A:154:CYS:HB2	2.15	0.47
1:A:156:LEU:CB	1:A:229:VAL:HG13	2.43	0.47
1:A:546:TRP:O	1:A:547:GLU:HG2	2.15	0.47
1:A:137:LYS:N	1:A:137:LYS:HD2	2.30	0.47
1:A:368:GLU:O	1:A:369:SER:C	2.53	0.47
1:A:385:GLN:HE22	1:A:463:ASN:CG	2.17	0.47
1:A:523:LEU:O	1:A:526:ASN:HB3	2.14	0.47
1:A:599:PHE:CE2	1:A:601:LEU:HG	2.50	0.47
1:A:173:TYR:CD2	1:A:210:PRO:HB3	2.50	0.47
1:A:169:SER:HB2	1:A:244:TRP:CD1	2.49	0.47
1:A:86:ASP:OD1	1:A:86:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:O	1:A:126:ARG:HG3	2.16	0.46
1:A:399:VAL:C	1:A:400:LYS:HD2	2.36	0.46
1:A:380:LYS:HB2	1:A:596:TRP:CZ2	2.50	0.46
1:A:431:ILE:O	1:A:435:LEU:HD22	2.15	0.46
1:A:209:VAL:CG2	1:A:209:VAL:O	2.63	0.46
1:A:196:LEU:HD21	1:A:428:GLU:HG3	1.98	0.46
1:A:30:PHE:HZ	1:A:119:ILE:O	1.98	0.46
1:A:177:PRO:HG3	1:A:212:PHE:CZ	2.50	0.46
1:A:386:LYS:NZ	1:A:464:ASN:HA	2.31	0.46
1:A:560:ASP:HB3	1:A:609:LEU:HD11	1.97	0.46
1:A:59:HIS:O	1:A:60:GLU:HG2	2.15	0.46
1:A:352:ILE:O	1:A:356:GLN:HG3	2.15	0.46
1:A:166:ARG:CZ	1:A:244:TRP:CE2	2.99	0.46
1:A:431:ILE:HG22	1:A:435:LEU:CD2	2.45	0.46
1:A:174:LEU:N	1:A:175:PRO:CD	2.78	0.46
1:A:26:ILE:HG13	1:A:27:LYS:HE3	1.96	0.46
1:A:468:GLU:OE1	1:A:468:GLU:N	2.49	0.46
1:A:62:VAL:CG2	1:A:213:ASN:HD21	2.29	0.45
1:A:604:ARG:HB3	1:A:608:VAL:HG13	1.98	0.45
1:A:396:SER:HB2	1:A:405:THR:HG21	1.97	0.45
1:A:124:GLN:NE2	1:A:124:GLN:H	2.13	0.45
1:A:155:HIS:HB3	1:A:231:GLU:HG3	1.99	0.45
1:A:422:TYR:O	1:A:423:ARG:HD3	2.17	0.45
1:A:385:GLN:NE2	1:A:463:ASN:ND2	2.64	0.45
1:A:443:PHE:O	1:A:447:LYS:HB2	2.16	0.45
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.61	0.45
1:A:153:GLY:HA2	1:A:231:GLU:OE1	2.17	0.44
1:A:596:TRP:CD1	1:A:597:ASN:HB2	2.52	0.44
1:A:354:LYS:HE3	1:A:354:LYS:HB3	1.56	0.44
1:A:554:TYR:HA	1:A:594:PRO:HD3	1.99	0.44
1:A:78:ILE:CD1	1:A:147:ILE:HD12	2.48	0.44
1:A:67:LEU:HA	1:A:70:VAL:CG2	2.48	0.44
1:A:147:ILE:HG22	1:A:239:LEU:HD11	1.99	0.44
1:A:173:TYR:O	1:A:174:LEU:HD22	2.17	0.44
1:A:126:ARG:HB3	1:A:138:LEU:CD1	2.43	0.44
1:A:88:TYR:CD1	1:A:90:VAL:HG12	2.53	0.44
1:A:520:ASN:OD1	1:A:522:LEU:HD13	2.17	0.44
1:A:530:ILE:HD12	1:A:531:ASP:H	1.83	0.44
1:A:113:LEU:HD12	1:A:113:LEU:O	2.17	0.43
1:A:447:LYS:HE3	1:A:451:LYS:HZ3	1.83	0.43
1:A:547:GLU:HA	1:A:548:SER:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:GLU:HG2	1:A:462:GLU:H	1.54	0.43
1:A:547:GLU:HA	1:A:548:SER:HA	1.83	0.43
1:A:31:ASN:HB3	1:A:34:ILE:HG23	2.00	0.43
1:A:192:PHE:HA	1:A:193:PRO:HD2	1.82	0.43
1:A:413:ARG:HD2	1:A:509:MET:HB2	2.00	0.43
1:A:493:LEU:HD13	1:A:632:VAL:HG11	2.00	0.43
1:A:620:LYS:HD2	1:A:620:LYS:HA	1.74	0.43
1:A:414:TYR:HA	1:A:510:ASP:CG	2.38	0.43
1:A:121:TYR:CG	1:A:143:THR:HG22	2.53	0.43
1:A:220:VAL:O	1:A:222:PRO:HD3	2.18	0.43
1:A:450:ILE:CG2	1:A:469:LEU:HD21	2.49	0.43
1:A:157:LEU:C	1:A:157:LEU:HD23	2.39	0.43
1:A:503:ARG:NH1	1:A:625:ASP:OD1	2.52	0.43
1:A:411:LYS:O	1:A:412:ALA:HB2	2.19	0.43
1:A:279:LEU:HD22	1:A:279:LEU:N	2.34	0.42
1:A:62:VAL:CG2	1:A:67:LEU:HG	2.49	0.42
1:A:450:ILE:HG22	1:A:469:LEU:HD21	2.01	0.42
1:A:342:ILE:HG12	1:A:347:LEU:HD21	2.00	0.42
1:A:604:ARG:HB3	1:A:608:VAL:HG11	1.99	0.42
1:A:471:LEU:HB3	1:A:502:ILE:HD12	2.02	0.42
1:A:560:ASP:HB3	1:A:609:LEU:CD1	2.48	0.42
1:A:556:LEU:O	1:A:610:GLU:HA	2.19	0.42
1:A:289:ARG:CG	1:A:289:ARG:NH1	2.65	0.42
1:A:289:ARG:NH1	1:A:289:ARG:HG2	2.08	0.42
1:A:133:THR:HG21	1:A:168:ILE:HD11	2.00	0.42
1:A:610:GLU:HG3	3:A:663:HOH:O	2.20	0.42
1:A:261:GLU:HB2	1:A:265:ARG:NH1	2.34	0.42
1:A:613:LYS:HE3	1:A:614:TYR:HB3	2.01	0.42
1:A:503:ARG:NH1	1:A:503:ARG:CG	2.83	0.42
1:A:365:LEU:HD23	1:A:367:ILE:HG13	2.01	0.42
1:A:464:ASN:O	1:A:468:GLU:OE1	2.37	0.42
1:A:294:PHE:C	1:A:294:PHE:CD2	2.92	0.42
1:A:447:LYS:HD3	1:A:469:LEU:HD22	2.02	0.42
1:A:277:ASN:ND2	1:A:277:ASN:C	2.70	0.42
1:A:382:VAL:CG1	1:A:466:ASP:HB3	2.50	0.42
1:A:503:ARG:NH1	1:A:625:ASP:OD2	2.52	0.42
1:A:371:LEU:HB2	1:A:597:ASN:HD21	1.86	0.41
1:A:129:PHE:CD2	1:A:245:TYR:CE2	3.08	0.41
1:A:284:PHE:O	1:A:406:ALA:HA	2.18	0.41
1:A:173:TYR:CE2	1:A:210:PRO:HB3	2.55	0.41
1:A:62:VAL:HG23	1:A:67:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CE2	1:A:245:TYR:HE2	2.38	0.41
1:A:163:ILE:O	1:A:164:GLY:C	2.58	0.41
1:A:511:PHE:HE2	1:A:513:LEU:HD11	1.85	0.41
1:A:586:ASP:OD1	1:A:586:ASP:C	2.58	0.41
1:A:591:ASN:O	1:A:593:PRO:HD3	2.20	0.41
1:A:294:PHE:CD2	1:A:295:HIS:N	2.88	0.41
1:A:472:ILE:O	1:A:476:VAL:HG23	2.21	0.41
1:A:158:THR:HA	1:A:228:ASP:HB3	2.03	0.41
1:A:414:TYR:HB3	1:A:510:ASP:HB3	2.02	0.41
1:A:70:VAL:HG12	1:A:113:LEU:HA	2.03	0.41
1:A:87:ILE:HG12	1:A:87:ILE:H	1.48	0.41
1:A:451:LYS:HE2	1:A:451:LYS:HB3	1.77	0.41
1:A:202:SER:HA	1:A:409:PRO:CG	2.21	0.41
1:A:414:TYR:HA	1:A:510:ASP:OD1	2.21	0.41
1:A:26:ILE:C	1:A:27:LYS:HE3	2.40	0.41
1:A:516:LYS:HG3	1:A:609:LEU:HD23	2.03	0.41
1:A:129:PHE:O	1:A:133:THR:HB	2.21	0.41
1:A:124:GLN:HE21	1:A:124:GLN:H	1.69	0.41
1:A:486:TYR:CZ	1:A:490:LEU:HD21	2.56	0.41
1:A:150:TYR:OH	1:A:156:LEU:HB2	2.21	0.40
1:A:364:SER:CA	1:A:601:LEU:O	2.69	0.40
1:A:208:LEU:O	1:A:210:PRO:HD3	2.21	0.40
1:A:173:TYR:CE1	1:A:210:PRO:HG2	2.56	0.40
1:A:613:LYS:O	1:A:614:TYR:C	2.59	0.40
1:A:395:HIS:CD2	1:A:397:LYS:H	2.35	0.40
1:A:133:THR:HG21	1:A:168:ILE:HD13	2.03	0.40
1:A:512:THR:C	1:A:513:LEU:HD12	2.41	0.40
1:A:261:GLU:C	1:A:263:TRP:H	2.25	0.40
1:A:452:ILE:HA	1:A:452:ILE:HD12	1.95	0.40
1:A:157:LEU:CA	1:A:228:ASP:HB2	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	521/644 (81%)	472 (91%)	46 (9%)	3 (1%)	30 65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	GLY
1	A	212	PHE
1	A	369	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	487/582 (84%)	407 (84%)	80 (16%)	3 8

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	34	ILE
1	A	36	ASP
1	A	38	THR
1	A	43	LEU
1	A	62	VAL
1	A	64	ASP
1	A	67	LEU
1	A	72	LYS
1	A	81	THR
1	A	87	ILE
1	A	91	ASN
1	A	113	LEU
1	A	117	ARG
1	A	123	LYS
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	128	PHE
1	A	129	PHE
1	A	133	THR
1	A	137	LYS
1	A	138	LEU
1	A	151	THR
1	A	156	LEU
1	A	157	LEU
1	A	158	THR
1	A	169	SER
1	A	171	ILE
1	A	182	LYS
1	A	191	LEU
1	A	195	ILE
1	A	213	ASN
1	A	229	VAL
1	A	234	VAL
1	A	240	SER
1	A	261	GLU
1	A	263	TRP
1	A	264	VAL
1	A	266	ASN
1	A	277	ASN
1	A	289	ARG
1	A	332	GLU
1	A	342	ILE
1	A	347	LEU
1	A	349	SER
1	A	365	LEU
1	A	369	SER
1	A	371	LEU
1	A	382	VAL
1	A	390	GLN
1	A	396	SER
1	A	405	THR
1	A	417	ILE
1	A	424	ASN
1	A	435	LEU
1	A	440	LEU
1	A	442	ASN
1	A	447	LYS
1	A	451	LYS

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Mol	Chain	Res	Type
1	A	461	ARG
1	A	462	GLU
1	A	463	ASN
1	A	474	LEU
1	A	485	LYS
1	A	487	LEU
1	A	490	LEU
1	A	502	ILE
1	A	503	ARG
1	A	509	MET
1	A	512	THR
1	A	518	ARG
1	A	524	LYS
1	A	548	SER
1	A	586	ASP
1	A	588	VAL
1	A	597	ASN
1	A	604	ARG
1	A	608	VAL
1	A	610	GLU
1	A	628	MET
1	A	634	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	54	ASN
1	A	91	ASN
1	A	112	ASN
1	A	148	ASN
1	A	211	GLN
1	A	213	ASN
1	A	214	GLN
1	A	242	GLN
1	A	249	GLN
1	A	266	ASN
1	A	267	ASN
1	A	277	ASN
1	A	299	HIS
1	A	340	GLN
1	A	356	GLN

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Mol	Chain	Res	Type
1	A	358	GLN
1	A	366	GLN
1	A	385	GLN
1	A	390	GLN
1	A	395	HIS
1	A	424	ASN
1	A	442	ASN
1	A	478	HIS
1	A	597	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	533/644 (82%)	0.07	11 (2%) 67 56	45, 63, 100, 124	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	ASN	5.5
1	A	264	VAL	3.1
1	A	464	ASN	3.0
1	A	451	LYS	2.8
1	A	257	PRO	2.7
1	A	250	VAL	2.6
1	A	251	GLY	2.3
1	A	143	THR	2.2
1	A	163	ILE	2.0
1	A	164	GLY	2.0
1	A	440	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FE2	A	1501	1/1	0.96	0.22	0.35	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.